Chemistry

Rechargeable Lithium batteries are needed for high performance communication devices and palm computers. Conducting polymer materials have been developed to improve the durability and lifetime of these new batteries.

The Chemistry organization research focus is to advance the science of interfaces by developing new analytical methods, and to develop novel synthetic materials. Areas of research include mass spectrometry, polymers and industrial separations science, supercritical fluids, theoretical chemistry and thermodynamics, and specialty biomedical chemistry and ion mobility spectrometry.

More than 60 chemists pursue fundamental chemistry research and technology development to support Department of Energy missions and industry customer needs. The organization has a strong fundamental science focus resulting in peer-reviewed publication and science and technology advances. Novel instruments, processes and products are the natural progression of such work, enabling strong, applications-oriented research.

Mass Spectrometry

Researchers are advancing the state of the art in mass spectrometry instrumentation and its application. They are exploring the underlying chemistry and physics of the processes involved in thermal ionization and particle-induced desorption from the solid state, and relating the ion production to the chemistry present in and on the solid state for both types of processes. In addition, the chemical reactivity of gas-phase neutrals with molecular ions derived from the solid state via particle desorption is being studied to determine the extent and kinetics of these reactions. Instrument research and development activities include ion optics modeling, ion trap secondary ion mass spectrometry, high-temperature surface analysis, elevated pressure mass spectrometry, and Fourier Transform Ion Cyclotron Resonance mass spectrometry coupled with optical spectroscopy. The mass spectrometry team is widely known for fundamental contributions to the field of ion optics modeling that include SIMION—a computer program is used to design ion optical components for mass spectrometers, ion gauges and ion guns.

Polymer and Separations Sciences

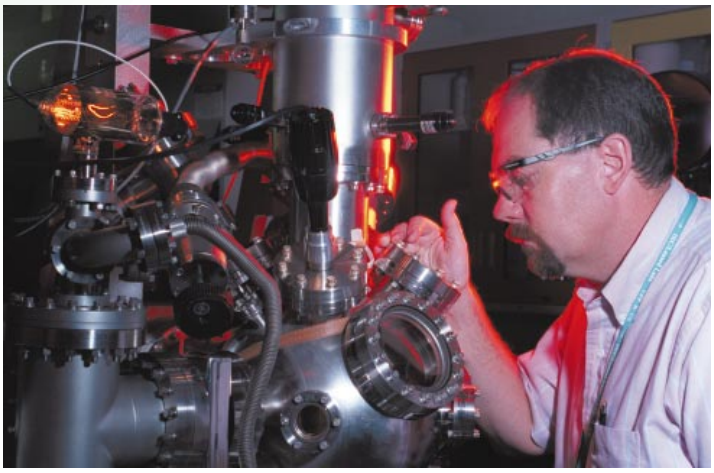
Researchers are developing new polymer membranes for a broad range of applications, including industrial separations. Fundamental research is focused on understanding the chemical and morphological properties of polymers, and the functional impact these characteristics have on separation performance. Examples of applications-oriented research include development of novel inorganic polymers based on phosphorous and nitrogen, battery electrolytes based on polyphosphazene polymers, and novel organic and inorganic sorbents for environmental pollutant abatement.

Supercritical Fluid

Researchers are working to better understand and harness the unique properties of supercritical fluids. Fundamental research focuses on understanding supercritical fluid solubility and solvent properties, and catalytic reactions at supercritical conditions. Applied research includes using supercritical fluids to enhance fossil fuel quality, remove low concentrations of actinides and fission products from soils, and developing technologies to make high-purity ultrafine particles at the production scale.

Continued on back

Attachment of chemical compounds to surfaces is being studied using advanced mass spectrometric methods to understand how chemicals interact with surfaces. Below, a special spectrometer is used to study the chemicals emitted from molten glass.



Idaho National Engineering and Environmental Laboratory
INEEL
Home of Science and Engineering Solutions

Continued from front

Theoretical Chemistry and Thermodynamics

Researchers focus on chemical phases, reactions and environments relevant to environmental restoration and immobilizing or degrading high-level waste in situ. Theoretical chemistry supports other focus areas in the Chemistry Department, and is prominent in the INEEL's Subsurface Science Initiative. A thorough understanding of molecular and electronic structure, thermodynamics and kinetics is critical to predicting the behavior of chemical species—including radioactive materials—in the subsurface.

Specialty Analytical Chemistry

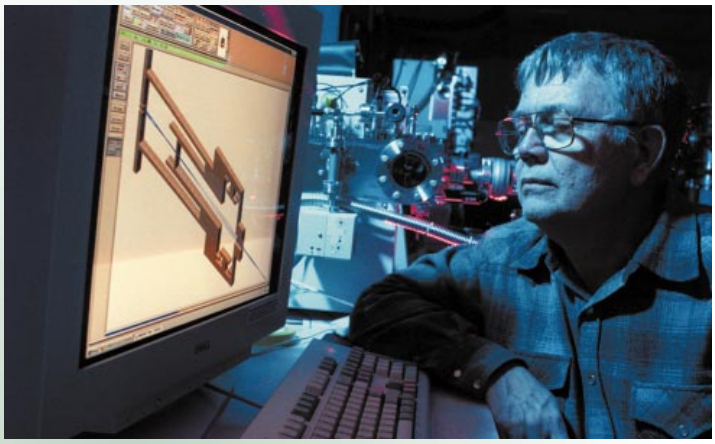
Researchers are developing new analytical chemistry methods and one-of-a-kind instruments for a range of applications. For example, scientists have developed total boron analysis methods for biological samples using a technique known as inductively-coupled plasma-atomic emission spectroscopy (ICP-AES). This research supports the development of boron neutron capture therapy, a cancer and arthritis treatment. Additionally, researchers are developing ion mobility measurement techniques to detect volatile, hazardous compounds.

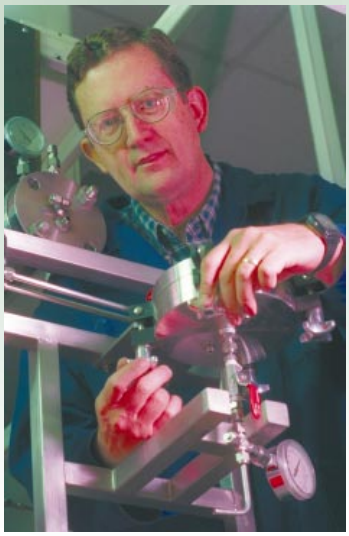
Support Chemistry

Chemists complement the research activities of other groups at the INEEL and provide technical support across the Laboratory and the world. Among the many efforts supported is the Sample Management Office, which provides services for the INEEL site to ensure the highest possible credibility on analyses that impact laboratory environmental programs.

The Chemistry organization supports a broad range of research for national laboratory and university partners, and other federal and industrial customers.

(clockwise starting at top) A novel ion source and mass spectrometer is being designed to operate at much higher pressures than commercial instruments. This instrument will be used to study how water interacts with ceramic surfaces. A compact ion mobility spectrometer is being constructed for detection of explosives, drugs and hazardous compounds. A membrane test cell is being configured to test new membrane materials for their ability to separate organic compounds from water.





Chemistry

Contacts:

Michael McIlwain, Ph.D.
(208) 526-8130
mem@inel.gov

David L. Miller, Ph.D.
(208) 526-9052
bsh@inel.gov

www.inel.gov/env-energyscience/chemistry